

1-Ethyl-2-methylbenzene
611-14-3 | DTXSID2050403

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.81 | 0.55 | 0.81 | 0.54 | 0.71 | 0.61 |

Model Results

Predicted value: 772 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.96e-01

Confidence level: 7.22e-01

Nearest Neighbors from the Training Set

Image not found

2,3,5-Trimethylphenol

Measured: 4070

Predicted: 345

Image not found

Propylbenzene

Measured: 741

Predicted: 859

Image not found

Ethylbenzene

Measured: 170

Predicted: 271

Image not found

1,2,3-Trimethylbenzene

Measured: 631

Predicted: 691

Image not found

1,3,5-Trimethylbenzene

Measured: 661

Predicted: 493